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On Extremal Bipartite Tricyclic Graphs

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Abstract

Let $\mathcal{T}_n^+$ be the set of connected bipartite tricyclic graphs with n vertices. Estrada and Higham proposed an invariant of a graph G based on Taylor series expansion of spectral moments $EE(G,c)=\sum_{k=0}^{\infty} c_k M_k(G)$. For $c_k=\frac{1}{k!}$ ($\frac{1}{n^k}$, $\frac{1}{(n-1)^k}$, respectively), $EE(G,c)$ is the Estrada index $EE(G)$ (Resolvent energy $ER(G)$, Resolvent Estrada index $EE_r(G)$, respectively) of G. The Kirchhoff index $Kf(G)$ of G is defined as $Kf(G)=\sum_{i<j} r_{ij}$, where r_{ij} is the effective resistance between vertices i and j in G. In this paper, the extremal graphs in $\mathcal{T}_n^+$ which have maximum, second-maximum $EE(G)$ ($ER(G)$, $EE_r(G)$ and $Kf(\bar{G})$, respectively) are determined.

1 Introduction

All graphs considered in this paper are finite and simple (i.e., without loops and multiple edges). For a graph G, let $V(G)=\{v_1,v_2,\ldots,v_n\}$ and $E(G)=\{e_1,e_2,\ldots,e_m\}$ denote the vertex set and edge set of the graph G, respectively. If $m=n-1+c$, then G is called a c-cyclic graph. If $c=0,1,2$ and 3, then G is a tree, unicyclic graph, bicyclic graph and tricyclic graph, respectively. For graph-theoretical terms that are not defined here, we refer to Bollobás's book [1].

For a graph G, the adjacency matrix of G, denoted by $A(G)$, is the sqare matrix (a_{ij}) in which $a_{ij}=1$ if the vertices v_i and v_j are adjacent, and $a_{ij}=0$ otherwise. The Laplacian matrix of G is the matrix $L(G)=D(G)-A(G)$ where $D(G)$ is a diagonal matrix with $(d_1,\ldots,d_n)$ on the main diagonal in which d_i is the degree of the vertex v_i. The characteristic polynomial $\phi(G;x))$ of G is defined as $\phi(G;x)=|xI-A(G)|$, and the

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Laplacian characteristic polynomial of G is defined as $\sigma(G;x) = |xI - L(G)|$, where I is the unit matrix. We denote the eigenvalues of $A(G)$ and $L(G)$ by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ and $\mu_1 \geq \ldots \geq \mu_{n-1} \geq \mu_n = 0$, respectively. Let $M_k(G)$ be the k-th spectral moment of a graph G, i.e., $M_k(G) = \sum_{i=1}^n \lambda_i^k$. It is well known that $M_k(G)$ is equal to the numbers of closed walks of length k in G.

In 1993, Klein and Randić [5] introduced a distance function named resistance distance on a graph. They view a connected graph G as an electrical network such that each edge of G is assumed to be a unit resistor, then take the resistance distance between vertices v_i and v_j to be the effective resistance between them, denoted by r_{ij}. The Kirchhoff index $Kf(G)$ of G [7] is defined as $Kf(G) = \sum_{i<j} r_{ij}$, and it is shown [4, 11] that

$$Kf(G) = \sum_{i<j} r_{ij} = n \sum_{i=1}^{n-1} \frac{1}{\mu_i} .$$

The Kirchhoff index has been investigated extensively in both mathematical and chemical literatures. For more information on the Kirchhoff index, the readers are referred to recent papers [13, 14, 16, 27, 29] and references therein.

The Estrada index of G, put forward by Estrada [21], is defined as $EE(G) = \sum_{i=1}^n e^{\lambda_i}$, and according to the Taylor series expansion of e^x, we have

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i} = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!} \tag{1.1}$$

Although invented in year 2000, the Estrada index has already found numerous applications. It was used to quantify the degree of folding of long-chain molecules, especially proteins [22, 24], and to measure the centrality of complex (communication, social, metabolic, etc.) networks [23, 25]. In addition, a connection between the Estrada index and the concept of extended atomic branching was found in [28]. Due to its extensive applications, the Estrada index has also been extensively studied in mathematics, and various mathematical properties of the Estrada index have been investigated (see [9, 10, 17, 18]).

The Resolvent Estrada index of G, proposed by Estrada and Higham in [26], is defined as $EE_r(G) = \sum_{i=1}^n \frac{n-1}{n-1-\lambda_i}$, where $G \neq K_n$. From the Taylor expansion, it is easy to see that

$$EE_r(G) = \sum_{i=1}^{n} \frac{n-1}{n-1-\lambda_i} = \sum_{k=0}^{\infty} \frac{M_k(G)}{(n-1)^k} \tag{1.2}$$

Quite recently, in analogy with the Resolvent Estrada index, the Resolvent Energy ER(G) of a graph G was introduced by I. Gutman et al. [12] as

$$ER(G) = \sum_{i=1}^{n} \frac{1}{n-\lambda_i} = \sum_{k=0}^{\infty} \frac{M_k(G)}{n^{k+1}} . \tag{1.3}$$

In 2010, Estrada and Higham [26] proposed a general formulation for the invariants of a graph G based on Taylor series expansion of spectral moments

$$EE(G,c)=\sum_{k=0}^{\infty}c_kM_k(G)\ .$$

Obviously, if the coefficient c_k takes $\frac{1}{k!}$, $\frac{1}{(n-1)^k}$ and $\frac{1}{n^{k+1}}$ then $EE(G,c)$ are the the Estrada index, Resolvent Estrada index and resolvent energy, respectively. Various properties of the Resolvent Estrada index and resolvent energy have been established [12, 19], and the indices for some special kinds of graphs, such as, trees, unicyclic graphs, random graphs etc., are also investigated.

In [15], Deng and Chen characterized the properties of the extremal connected bipartite unicyclic graphs based on the Estrada index of themselves and the Kirchhoff index of their complements. In [20], Huang et al. established the upper bound of the Estrada index and the Kirchhoff index of the connected bipartite bicyclic graphs. Here we study the four indices of the bipartite tricyclic graphs and wish to shed some light on the relationship between them.

2 Preliminaries

A graph G is called bipartite if its vertex set can be partitioned into two subsets X and Y so that every edge has one end in X and the other end in Y. Let P_n, C_n and S_n be the path, the cycle and the star on n vertices, respectively. Denote by $d_G(v)=|N_G(v)|$ the degree of the vertex v of G. If $E_0\subset E(G)$, we denote by $G-E_0$ the subgraph of G obtained by deleting the edges in E_0. If E_1 is the subset of the edge set of the complement of G, $G+E_1$ denotes the graph obtained from G by adding the edges in E_1. Similarly, if $W\subset V(G)$, we denote by $G-W$ the subgraph of G obtained by deleting the vertices of W and the edges incident with them.

For any vertices u,v and w (not necessarily distinct) in G, we denote by $M_k(G;u,v)$ the number walks in G with length k from u to v. Denote by $W_k(G;u,v)$ the walk set of length k from u to v in G. Clearly $M_k(G;u,v)=|W_k(G;u,v)|$. Note that $M_k(G;u,v)=M_k(G;v,u)$ for any positive integer k [3].

Let G and H be two graphs with $u_1,v_1\in V(G)$, $u_2,v_2\in V(H)$. If $M_k(G;u_1,v_1)\le M_k(H;u_2,v_2)$ for all positive integers k, then we write $(G;u_1,v_1)\preceq(H;u_2,v_2)$. If $(G;u_1,v_1)\preceq(H;u_2,v_2)$ and there is at least one positive integer k_0 such that $M_{k_0}(G;u_1,v_1)<M_{k_0}(H;u_2,v_2)$, then we write $(G;u_1,v_1)\prec(H;u_2,v_2)$.

Let G be a simple graph with n vertices and m edges and put $S(G)$ to be the subdivision graph of G, that is, the graph obtained from G by inserting a new vertex in each edge of G. By [2], we have

$$\phi(S(G); x) = x^{m-n}\sigma(G; x^2) \ . \tag{2.4}$$

Lemma 2.1. *Let $G(G \neq K_n)$ be a connected graph with n vertices, then*

$$ER(G) = \frac{\phi'(G,n)}{\phi(G,n)} \qquad EE_r(G) = (n-1)\frac{\phi'(G,n-1)}{\phi(G,n-1)}$$

where $\phi'(G,x)$ is the first derivative of $\phi(G,x)$.

Proof. Let $\lambda_1; \lambda_2; \cdots; \lambda_n$ be the eigenvalues of G, then $\phi(G,x) = (x-\lambda_1)(x-\lambda_2)\cdots(x-\lambda_n)$. The equations follow from the definition (1.3) and (1.2) by taking into account $x = n$ and $x = n-1$, respectively. ∎

Lemma 2.2 ([16])**.** *Let $\overline{G}$ be the connected complement graph of a graph G. Then*

$$Kf(\overline{G}) = n\frac{\sigma'(G,n)}{\sigma(G,n)} - 1$$

Lemma 2.3 ([16])**.** *Let G be a bipartite graph with $n(n \geq 2)$ vertices and m edges. Then*

$$Kf(\overline{G}) = \frac{n-m}{2} + \frac{1}{2}\sum_{k=0}^{\infty}\frac{M_{2k}(S(G))}{n^k} - 1 \ .$$

Let $\mathcal{T}_n^+$ be the set of all bipartite tricyclic graphs with n vertices. For any graph $G \in \mathcal{T}_n^+$, since G is a bipartite graph with $m = n+2$, from the Lemma 2.3, it follows

$$Kf(\overline{G}) = \frac{1}{2}\sum_{k=0}^{\infty}\frac{M_{2k}(S(G))}{n^k} - 2 \tag{2.5}$$

Remark 1. In view of (1.1)-(1.3) and (2.5), $EE(G)$, $ER(G)$, $EE_r(G)$and $Kf(\overline{G})$ have certain similarity. That is, for $G, H \in \mathcal{T}_n^+$ (in this case $M_{2k-1}(G) = M_{2k-1}(H) = 0$), if $M_{2k}(G) \geq M_{2k}(H)$ for all positive integers k, then $EE(G) \geq EE(H), ER(G) \geq ER(H)$ and $EE_r(G) \geq EE_r(H)$. Furthermore, with equality if and only if $M_{2k}(G) = M_{2k}(H)$ for all positive integers k, and the same thing is true for $Kf(\overline{G})$ and $Kf(\overline{H})$ by considering the number of closed walks in $S(G)$ instead of those in G.

Lemma 2.4 ([3])**.** *Let v be a vertex of a graph G, and $C(v)$ be the set of all cycles containing v. Then the characteristic polynomial of G satisfies*

$$\phi(G; x) = x\phi(G-v; x) - \sum_{uv \in E(G)}\phi(G-u-v; x) - 2\sum_{Z \in C(v)}\phi(G \setminus V(Z); x) \ .$$

here $\phi(G-u-v; x) = 1$ if G is a single edge,and $\phi(G \setminus V(Z); x) = 1$ if G is a cycle.

Lemma 2.5 ([8]). *Let H be a graph (not necessarily connected) with $u, v \in V(H)$. Suppose that $w_i \in V(H)$, and $uw_i, vw_i \notin E(H)$ for $i = 1, 2, \ldots, r$, where r is a positive integer. Let $E_u = \{uw_1, uw_2, \ldots, uw_r\}$ and $E_v = \{vw_1, vw_2, \ldots, vw_r\}$. Let $H_u = H + E_u$ and $H_v = H + E_v$. If $(H; u, u) \prec (H; v, v)$ and $(H; w_i, u) \preceq (H; w_i, v)$ for $1 \le i \le r$, then $M_k(H_u) \le M_k(H_v)$ for all positive integers k and it is strict for some positive integer k_0.*

The coalescence of two vertex-disjoint connected graphs G, H, denoted by $G(u) \circ H(w)$, where $u \in V(G)$ and $w \in V(H)$, is obtained by identifying the vertex u of G with the vertex w of H. Let A, B, C be three connected graphs, and each of which has at least two vertices. Let u, v be two different vertices of C, u' a vertex of A (v' a vertex of B), then we define

$$H = A(u') \circ C(u); \quad G = H(v) \circ B(v'); \quad G' = H(u) \circ B(v'),$$

where the vertex u in H denotes the corresponding vertex of the coalescence of u' in A and u in C (see Fig.1). Then we have the following results.

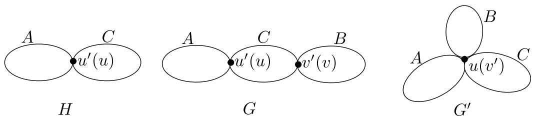

Figure 1. The graphs G and G'.

Lemma 2.6 ([15]). *For the notation as above. Suppose that there exists an automorphism φ of C such that $\varphi(u) = v$, then:*
(i)$(H; u, u) \succ (H; v, v)$, that is, $M_k(H; u, u) \ge M_k(H; v, v)$ for all positive integer k and it is strict for some positive integer k_0.
(ii)$M_k(G') \ge M_k(G)$for positive integer k and it is strict for some positive integer k_0.

Remark 2. It is clear that, if C is a path, then C naturally satisfies the condition of Lemma 2.6, thus the application of Lemma 2.4 makes the number of closed walks of length k increase, that is, $M_k(G') \ge M_k(G)$. Further, if A, B are trees and C is a path, then G' is just the graph obtained from G by a proper generalized tree shift(GTS) defined in [6]. Therefore, a direct consequence of Lemma 2.6 is that the proper GTS increases the number of closed walks of length k.

Lemma 2.7 ([18]). *Let H_1 be a connected graph containing two vertices u, v, and let H_2 be a connected graph disjoint to H_1, which contains a vertex w. Let H_2' be a copy of H_2, containing the vertex w' corresponding to w of H_2. Let $G = (H_1(u) \circ H_2(w))(v) \circ H_2'(w')$.*

(i) *If there exists an automorphism* σ *of* H_1 *such that it interchanges* u *and* v*, then* $(G;u,t) = (G;v,\sigma(t))$ *for any vertex* t.

(ii) *If letting* $\bar{H}_1$ *be obtained from* H_1 *by adding some edges incident with* v *but not* u*, letting* $\bar{H}_2$ *be obtained from* H_2' *by adding some vertices or edges such that the resulting graph is connected, and letting* $\bar{G}$ *be obtained from* G *by replacing* H_1 *with* $\bar{H}_1$ *or* H_2' *with* $\bar{H}_2$*, then* $(\bar{G};u,t) \prec (\bar{G};v,\sigma(t))$.

3 Maximum indices of bipartite tricyclic graphs

In this section we find extremal graphs in $\mathcal{T}_n^+$ for the Estrada index $EE(G)$, Resolvent Estrada index $EE_r(G)$, Resolvent Energy $ER(G)$ and Kirchhoff index $Kf(\overline{G})$, respectively. For a graph $G \in \mathcal{T}_n^+$, the base of G, denoted by $B(G)$, is the minimal connected bipartite tricyclic subgraph of G. Obviously, $B(G)$ is the unique bipartite tricyclic subgraph of G containing no pendant vertex, and G can be obtained from $B(G)$ by planting trees to some vertices of $B(G)$. Since each tree can be transformed into a star by a sequence of applications of Lemma 2.6, and the k-th spectral moment M_k is monotone in the course of the transformation. Therefore, the extremal graph with the maximal indices is obtained from the graphs in which the attaching trees to the base are all stars. In the following discussion, we consider the graphs of $\mathcal{T}_n^+$ with the base by attaching pendent vertices.

According to [30] and [31], we know that bipartite tricyclic graphs have many kinds of bases. By applying Lemma 2.6 and Remark 2 repeatedly, we get the lemma.

Lemma 3.1. *If* G *is an extremal graph with maximum* $EE(G)$ *(*$EE_r(G)$*,* $ER(G)$ *or* $Kf(\overline{G})$*) in* $\mathcal{T}_n^+$*, then* $B(G) \cong T_n^j, j \in \{1,2,\cdots,7\}$*. (see Fig.2).*

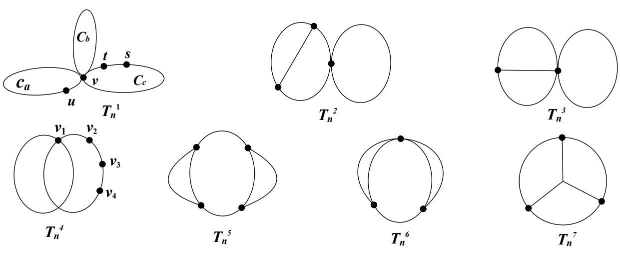

Figure 2. The graphs $T_n^j (j = 1,2,3,4,5,6,7)$.

Lemma 3.2. *For any graph G with the base $B(G) \cong T_n^1$, there exists a graph G' with the base $B(G') \cong T_n^3$ such that $EE(G) < EE(G')$ $EE_r(G) < EE_r(G')$, $ER(G) < ER(G')$, $Kf(\overline{G}) < Kf(\overline{G'})$, respectively.*

Proof. Let u, v, t, s be the vertices of G (as shown in Fig.2), without loss of generality, let $d_G(u) \geq d_G(s)$, $H = G - ts$ and $G' = H + us$.

For any closed walk $W \in W_k(H; t, t)$, if it does not go through the vertex v, then let $f(W)$ be the walk obtained from W by replacing every t and its pendent vertices in W by u and its corresponding pendent vertices, respectively. Otherwise, the closed walk W is decomposed into three sections W_1, W_2, W_3, where W_1 is the shortest (t, v)-section at the beginning of W, W_2 is the longest (v, v)-section in the middle of W, and the remaining (v, t)-section is W_3. In this case, let $f(W)$ be the walk obtained from W by replacing every t and its pendent vertices in $W_1 \cup W_2$ by u and its corresponding pendent vertices, respectively, and W_2 remain the same. Obviously, $f(W) \in W_k(H; u, u)$ and f is an injection from $W_k(H; t, t)$ to $W_k(H; u, u)$, i.e., $M_k(H; t, t) \leq M_k(H; u, u)$. Furthermore, $M_2(H; t, t) < M_2(H; u, u)$. It implies that $(H; t, t) \prec (H; v, v)$.

For any walk $W' \in W_k(H; t, s)$, W' can be decomposed into two sections W_1', W_2', where W_1' is the shortest (t, v)-section of W', and W_2' is the remaining (v, s)-section. In this case, let $g(W')$ be the walk obtained from W' by replacing every t and its pendent vertices in W_1' by u and its corresponding pendent vertices, respectively, and W_2' remain the same. Obviously, $g(W') \in W_k(H; u, s)$ and g is an injection from $W_k(H; t, s)$ to $W_k(H; u, s)$, i.e., $M_k(H; t, s) \leq M_k(H; u, s)$. Considering that $G = H + ts$ and $G' = H + us$, by Lemma 2.5 we have $EE(G) < EE(G')$ ($EE_r(G) < EE_r(G')$, $ER(G) < ER(G')$).

Let $S(G)$ and $S(G')$ be the subdivisions of G and G', respectively, and let $B = S(G) - tv_{ts}$, where v_{ts} denotes the subdividing vertex of the edge ts. Note that $S(G) = B + tv_{ts}$ and $S(G') = B + uv_{ts}$. Then in a similar way, applying Lemma 2.5, we have $Kf(\overline{G}) < Kf(\overline{G'})$. ■

Similar to the proof of Lemma 3.2, we have the following lemma.

Lemma 3.3. *For any graph G with the base $B(G) \cong T_n^i (i \in \{2, 3\})$, there exists a graph G' with the base $B(G') \cong T_n^j (j \in \{4, 5, 6\})$ such that $EE(G) < EE(G')$ ($EE_r(G) < EE_r(G')$, $ER(G) < ER(G')$, $Kf(\overline{G}) < Kf(\overline{G'})$).*

Corollary 3.4. *If G is an extremal graph with maximal $EE(G)$ ($EE_r(G)$, $ER(G)$ or $Kf(\overline{G})$) in $\mathcal{T}_n^+$, then $B(G) \cong T_n^j, j \in \{4, \cdots, 7\}$*

Lemma 3.5. *If $G \in \mathcal{T}_n^+$ is an extremal graph with maximum indices, and $B(G) \cong T_n^j, j \in \{4, \cdots, 7\}$, then there are no three successive 2-degree vertices on each cycle of the base $B(G)$ of G.*

Proof. Suppose there exist three successive 2-degree vertices on a cycle of the base $B(G)$ of G. Without loss of generality, let $B(G) \cong T_n^4$ and $d_G(v_1) \geq d_G(v_4)$ (as shown in Figure 2), where v_2, v_3, v_4 are 2-degree vertices of $B(G)$. Let $H = G - v_3v_4$, $G' = H + v_1v_4$.

For any closed walk $W \in W_k(H; v_3, v_3)$, if it does not go through the vertex v_2, then let $f(W)$ be the walk obtained from W by replacing every v_3 and its pendent vertices in W by v_1 and its corresponding vertices of $N_G(v_1)$, respectively. Otherwise, the closed walk W is decomposed into three sections W_1, W_2, W_3, where W_1 is the shortest (v_3, v_2)-section at the beginning of W, W_2 is the longest (v_2, v_2)-section in the middle of W, and the remaining (v_2, v_3)-section is W_3. In this case, let $f(W)$ be the walk obtained from W by replacing every v_3 and its pendent vertices in $W_1 \cup W_3$ by v_1 and its corresponding vertices of $N_G(v_1)$, respectively, and W_2 remain the same. Obviously, $f(W) \in W_k(H; v_1, v_1)$ and f is an injection from $W_k(H; v_3, v_3)$ to $W_k(H; v_1, v_1)$, i.e., $M_k(H; v_3, v_3) \leq M_k(H; v_1, v_1)$. Furthermore, $M_2(H; v_3, v_3) < M_2(H; v_1, v_1)$. It implies that $(H; v_3, v_3) \prec (H; v_1, v_1)$.

For any walk $W' \in W_k(H; v_3, v_4)$, W' can be decomposed into two sections W_1', W_2', where W_1' is the shortest (v_3, v_2)-section of W', and W_2' is the remaining (v_2, v_4)-section. In this case, let $g(W')$ be the walk obtained from W' by replacing every v_3 and its pendent vertices in W_1' by v_1 and its corresponding vertices of $N_G(v_1)$, respectively, and W_2' remain the same. Obviously, $g(W') \in W_k(H; v_1, v_4)$ and g is an injection from $W_k(H; v_3, v_4)$ to $W_k(H; v_1, v_4)$, i.e., $M_k(H; v_3, v_4) \leq M_k(H; v_1, v_4)$. Considering that $G = H + v_3v_4$ and $G' = H + v_1v_4$, by the lemma 2.5, we have $EE(G) < EE(G')$ ($EE_r(G) < EE_r(G')$, $ER(G) < ER(G')$) and $B(G') \cong T_n^4$. This contradicts the condition of Lemma 3.5.

Similarly, Let $S(G)$ be the subdivisions of G, and let $H' = S(G) - v_3v_{34}$ and $S(G') = H + v_1v_{34}$, where v_{34} denotes the subdividing vertex of the edge v_3v_4. Note that $S(G) = H' + v_3v_{34}$. Applying the similar way, and by Lemma 2.5, we have $Kf(\overline{G}) < Kf(\overline{G'})$, contradiction. ■

The internal path of G is a walk $v_0v_1 \ldots v_s$ such that the vertices $v_0, v_1, \ldots, v_s$ are distinct, $d_G(v_0) > 2, d_G(v_s) > 2$, and $d_G(v_i) = 2$, whenever $0 < i < s$.

Lemma 3.6. *Let $G \in \mathcal{T}_n^+$, and $B(G) \in T_n^i (i = 4, 5, 6, 7)$, $P_u^k = uv_1v_2$ and $P_u^l = uw_1w_2$ be two internal path in $B(G)$, where $d_{B(G)}(u) \geq 3$ $(u \in B(G))$, if $v_2 \neq w_2$, then there exists a graph $G'(B(G') \in T_n^i (i = 4, 5, 6, 7))$ such that $|E(B(G))| - |E(B(G'))| = 1$ and $EE(G) < EE(G')$ ($EE_r(G) < EE_r(G')$, $ER(G) < ER(G')$ or $Kf(\overline{G}) < Kf(\overline{G'})$).*

Proof. Without loss of generality, let $d_G(w_1) \geq d_G(v_1)$, $H = G - v_1v_2$, and let $G' = H + w_1v_2$. By the same way mentioned above, we obtain $(H; v_1, v_1) \prec (H; w_1, w_1)$ and $M_k(H; v_1, v_2) \leq M_k(H; w_1, v_2)$. Obviously, G' is still bipartite tricyclic graph, and $|E(B(G))| - |E(B(G'))| = 1$. According to the lemma 2.5, the result holds. ■

By the lemma 3.5 and lemma 3.6, we have the following result.

Corollary 3.7. *If G is the graph with maximum $EE(G)(EE_r(G), ER(G)$ or $Kf(\overline{G}))$, and $B(G) \in T_n^i(i = 4, 5, 6, 7)$. Then $B(G) \in A_1 \cup A_2$ (as shown in Fig. 3).*

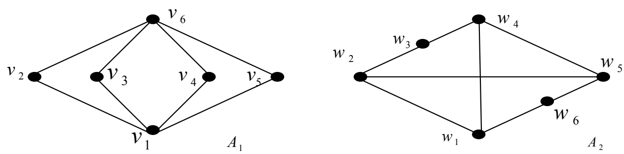

Figure 3. The graphs $A_j (j = 1, 2)$.

Lemma 3.8. *If G is the graph with maximum $EE(G)$ $(EE_r(G), ER(G)$ or $Kf(\overline{G}))$ and $B(G) \cong A_i, i \in \{1, 2\}$ (see Fig. 3), then G is obtained from A_i by attaching $n - |V(A_i)|$ pendent vertices at a vertex v_1 with maximum degree in $A_i (i \in \{1, 2\})$.*

Proof. For the case of $B(G) \cong A_1$, let $\{v_1, v_2, v_3, v_4, v_5, v_6\}$ be the vertices of A_1 as shown in Fig 3, and let n_i $(n_i \geq 0)$ be the pendant vertices attached to v_i in G, $i = 1, 2, 3, 4, 5, 6$. For convenience, we denote $G = A_1(n_1, n_2, n_3, n_4, n_5, n_6)$.

First of all, it can be claimed that at least three numbers of n_2, n_3, n_4, n_5 are zero. If not so, we put $n_2 > 0, n_3 > 0$, and let H be the graph obtained from $A_1(n_1, n_2, n_3, 0, 0, n_6)$ by deleting n_2 and n_3 pendent vertices of v_2 and v_3, respectively. Then there exists an automorphism of H which interchanges v_2, v_3 and preserves all other vertices. Based on Lemma 2.6 (ii), we have

$$M_{2k}(A_1(n_1, n_2, n_3, 0, 0, n_6)) \leq M_{2k}(A_1(n_1, n_2 + n_3, 0, 0, 0, n_6)) \ .$$

Let $S(H)$ be the subdivision graph of H, similar to the analysis, one can easily obtain the following result.

$$M_{2k}(S(A_1(n_1, n_2, n_3, 0, 0, n_6))) \leq M_{2k}(S(A_1(n_1, n_2 + n_3, 0, 0, 0, n_6))) \ .$$

This contradicts the condition of Lemma 3.8. Similarly, we can confirm that at least one number of n_1, n_6 is zero.

Table 1. The Estrada index of graphs T_1, T_2 for $6 \leq n \leq 15$.

	$n=6$	$n=7$	$n=8$	$n=9$	$n=10$	$n=11$	$n=12$	$n=13$	$n=14$	$n=15$
$EE(T_1)$	20.978	24.098	27.492	31.186	35.205	39.579	44.335	49.508	55.129	61.236
$EE(T_2)$	21.990	24.827	27.914	31.275	34.934	38.916	43.251	47.967	53.097	58.675

Without loss of generality, let $n_3 = 0, n_4 = 0, n_5 = 0$ and $n_6 = 0$, then $G = A_1(n_1, n_2, 0, 0, 0, 0)$. If both n_1, n_2 are nonzero, let H_1 be the graph obtained from A_1 by deleting the edges v_1v_3, v_1v_4 and the pendent vertices of v_2 and v_1, respectively. Then there exists an automorphism which interchanges v_1, v_2 and preserves all other vertices, and let H_1' be the graph obtained from H_1 by adding the edges v_1v_3, v_1v_4 and the pendent vertices of v_1. It is clear that $M_2(H_1'; v_2, v_2) = 2 < 4 + n_1 = M_2(H_1'; v_1, v_1)$. By Lemma 2.6 (ii), we have $(H_1'; v_2, v_2) \prec (H_1'; v_1, v_1)$. Further by Lemma 2.5,

$$M_{2k}(A_1(n_1, n_2, 0, 0, 0, 0)) \leq M_{2k}(A_1(n_1 + n_2, 0, 0, 0, 0)) \ .$$

By the same way, we can deduce the following inequality

$$M_{2k}(S(A_1(n_1, n_2, 0, 0, 0, 0))) \leq M_{2k}(S(A_1(n_1 + n_2, 0, 0, 0, 0))),$$

this contradicts to the hypothesis of lemma 3.8. The proof is completed for the case of $B(G) \cong A_1$. Similarly, we can prove the case for $B(G) \cong A_2$. ■

Let $T_1 = A_1(n-6, 0, 0, 0, 0, 0)$, $T_2 = A_2(n-6, 0, 0, 0, 0, 0)$, by Lemma 2.4, we have

$$\begin{aligned}
\phi(T_1; x) &= x^{n-4}[x^4 - (n+2)x^2 + 4(n-6)] = x^{n-4} f_1(x) \, ; \\
\phi(T_2; x) &= x^{n-6}[x^6 - (n+2)x^4 + (5n-26)x^2 - 2(n-6)] = x^{n-6} f_2(x) \ .
\end{aligned}$$

Furthermore, from the Lemma 2.4 and the equation (2.4), it follows that

$$\begin{aligned}
\sigma(T_1; x) &= (x-2)^2(x-1)^{n-7}[x^5 - (n+7)x^4 + (8n+8)x^3 \\
&\quad +(4-16n)x^2 + (6+8n)x - 6] = (x-2)^2(x-1)^{n-7} g_1(x) \, ; \qquad (3.6) \\
\sigma(T_2; x) &= x(x-1)^{n-7}[x^6 - (n+11)x^5 + (13n+36)x^4 - (62n+14)x^3 \\
&\quad +(133n-5)x^2 + (117-123n)x + 36n] = x(x-1)^{n-7} g_2(x) \ . \qquad (3.7)
\end{aligned}$$

Theorem 3.9. *Let G be a graph in $\mathcal{T}_n^+$,*

(i) *If $6 \leq n \leq 9$, then $EE(G) \leq EE(T_2)$ with equality if and only if $G \cong T_2$; If $n \geq 10$, then $EE(G) \leq EE(T_1)$ with equality if and only if $G \cong T_1$.*

(ii) *For each* n $(n \geq 6)$*,* $ER(G) \leq ER(T_1)$ *and* $EE_r(G) \leq EE_r(T_1)$ *with equality if and only if* $G \cong T_1$*.*

(iii) *For each* n $(n \geq 6)$*,* $Kf(\overline{G}) \leq Kf(\overline{T_1})$ *with equality if and only if* $G \cong T_1$*.*

Proof. (i) Obviously, according to the table 1, the result holds for $6 \leq n \leq 9$. For the case $n \geq 10$, by calculation using software Matlab, we can see that the result is true for the integer $n(10 \leq n \leq 100)$. In the following discussion, we let $n > 100$.

We know that the solutions of $f_1(x) = 0$ are $\pm\sqrt{\frac{n+2+\sqrt{n^2-12n+100}}{2}}, \pm\sqrt{\frac{n+2-\sqrt{n^2-12n+100}}{2}}$ and the graph $T_1 - v_1$ has eigenvalues ± 2, 0 with multiplicity $n-3$. By interlacing property of eigenvalues, $\lambda_i(T_1) \geq \lambda_i(T_1 - v_1)$ for $i = 2, 3, \ldots, n-1$ [3]. Then

$$\begin{aligned} EE(T_1) &= \sum_{i=1}^{n} e^{\lambda_i(T_1)} > e^{\lambda_1(T_1)} + \sum_{i=2}^{n-1} e^{\lambda_i(T_1 - v_1)} + e^{\lambda_n(T_1)} \\ &> e^{\sqrt{\frac{n+2+\sqrt{n^2-12n+100}}{2}}} + (n-3) + e^{-2} + 1 \\ &> e^{\sqrt{n-2}} + (n-2) + e^{-2} = H_1 \end{aligned}$$

By a direct calculation, the graph $T_2 - v_1$ has eigenvalues $\pm\sqrt{\frac{5+\sqrt{17}}{2}}, \pm\sqrt{\frac{5-\sqrt{17}}{2}}$, 0 with multiplicity $n-5$. For $n \geq 101$,

$$f_2\left(\sqrt{n - \frac{5}{2}}\right) = \frac{1}{2}\left(n^2 - 36n + \frac{391}{4}\right) > 0\,, \qquad f_2(\sqrt{n-3}) = -13n - 45 < 0$$

Because of the fact $\lambda_1(T_2) \geq \lambda_1(T_2 - v_1)$, we have $\sqrt{\frac{5+\sqrt{17}}{2}} \leq \lambda_1(T_2) < \sqrt{n - \frac{5}{2}}$. By interlacing property of eigenvalues of $T_2 - v_1$ and T_2, $\lambda_i(T_2) \leq \lambda_{i-1}(T_2 - v_1)$ for $i = 2, 3, \ldots, n$, then

$$\begin{aligned} EE(T_2) &= \sum_{i=1}^{n} e^{\lambda_i(T_2)} \leq e^{\lambda_1(T_2)} + \sum_{i=1}^{n-1} e^{\lambda_i(T_2 - v_1)} \\ &< e^{\sqrt{n-\frac{5}{2}}} + (n-5) + e^{\sqrt{\frac{5+\sqrt{17}}{2}}} + e^{-\sqrt{\frac{5+\sqrt{17}}{2}}} + e^{\sqrt{\frac{5-\sqrt{17}}{2}}} + e^{-\sqrt{\frac{5-\sqrt{17}}{2}}} = H_2\,. \end{aligned}$$

Note that $e^{\sqrt{n-2}} - e^{\sqrt{n-\frac{5}{2}}} + e^{-2} + 1 - e^{\sqrt{\frac{5+\sqrt{17}}{2}}} - e^{\sqrt{\frac{5-\sqrt{17}}{2}}} > 0$ for $n \geq 32$, then $H_1 - H_2 > 0$. Therefore $EE(T_1) > EE(T_2)$.

(ii) By Lemma 2.1, it follows that

$$\begin{aligned} ER(T_1) - ER(T_2) &= \frac{\phi'(T_1, n)}{\phi(T_1, n)} - \frac{\phi'(T_2, n)}{\phi(T_2, n)} \\ &= \frac{\phi'(T_1, n)\phi(T_2, n) - \phi'(T_2, n)\phi(T_1, n)}{\phi(T_1, n)\phi(T_2, n)} \\ &= \frac{(n-2)(4n^6 - 2n^5 - 16n^4 + 56n^3 + 80n^2 + 48n + 288)}{nf_1(n)f_2(n)} \end{aligned}$$

The real roots of the polynomials $f_1(n) = n^4 - n^3 - 2n^2 + 4n - 24$ and $f_2(n) = n^6 - n^5 - 2n^4 + 5n^3 - 26n^2 - 2n + 12$ are less than 3, thus the denominator is positive for $n \geq 3$. On the other hand, the polynomial $p(n) = 4n^6 - 2n^5 - 16n^4 + 56n^3 + 80n^2 + 48n + 288$ does not have any real roots, therefore, the numerator is positive for $n \geq 3$. It implies that $ER(T_1) \geq ER(T_2)$.

Similarly, from the Lemma 2.1, it follows that

$$\begin{aligned}
EE_r(T_1) - EE_r(T_2) &= (n-1)\left(\frac{\phi'(T_1, n-1)}{\phi(T_1, n-1)} - \frac{\phi'(T_2, n-1)}{\phi(T_2, n-1)}\right) \\
&= (n-1)\left(\frac{\phi'(T_1, n-1)\phi(T_2, n-1) - \phi'(T_2, n-1)\phi(T_1, n-1)}{\phi(T_1, n-1)\phi(T_2, n-1)}\right) \\
&= \frac{4n^7 - 34n^6 + 104n^5 - 76n^4 - 212n^3 + 342n^2 + 72n - 600}{f_1(n-1)f_2(n-1)}
\end{aligned}$$

Where $f_1(n-1) = n^4 - 5n^3 + 6n^2 + 3n - 25$, $f_2(n-1) = n^6 - 7n^5 + 17n^4 - 13n^3 - 29n^2 + 56n - 15$, since the real roots of the polynomials $f_1(n-1)$ and $f_2(n-1)$ are less than 4, then the denominator is positive for $n \geq 4$. In the meantime, the numerator is positive for $n \geq 3$. It follows that $EE_r(T_1) \geq EE_r(T_2)$.

(iii) From Lemma 2.2, Eqs.(3.6) and (3.7), we have

$$\begin{aligned}
Kf(\overline{T_1}) - Kf(\overline{T_2}) &= n\left(\frac{\sigma'(T_1, n)}{\sigma(T_1, n)} - \frac{\sigma'(T_2, n)}{\sigma(T_2, n)}\right) \\
&= n\left(\frac{\sigma'(T_1, n)\sigma(T_2, n) - \sigma'(T_2, n)\sigma(T_1, n)}{\sigma(T_1, n)\sigma(T_2, n)}\right) \\
&= \frac{n^{11} - 32n^{10} + 412n^9 - 2678n^8 + 9445n^7 - 17942n^6 + \cdots + 3240}{(n-1)(n-2)g_1(n)g_2(n)}
\end{aligned}$$

Where $g_1(n) = n^4 - 8n^3 + 12n^2 + 6n - 6$, $g_2(n) = 2n^5 - 26n^4 + 119n^3 - 128n^2 + 153n$, since the real roots of the polynomials $g_1(n)$ and $g_2(n)$ are less than 6, then the denominator is positive for $n \geq 6$. By direct calculation, the numerator is positive for $n \geq 3$. It follows that $Kf(\overline{T_1}) \geq Kf(\overline{T_2})$.

This completes the proof. ■

4 The second maximum indices of bipartite tricyclic graphs

In this section, we will consider the graphs with the second maximum $EE(G)$, $ER(G)$, $EE_r(G)$ or $Kf(\overline{G})$ among T_n^+. By Corollary 3.7, Lemma 2.6 and Theorem 3.9, one can conclude that G which has the second maximum indices of bipartite tricyclic graphs must be one of the graphs $A_1(n_1, n_2, 0, 0, 0, 0)$, $A_1(n_1, 0, 0, 0, 0, n_6)$, T_5, T_6, T_7 (as shown in Fig.4) and T_2.

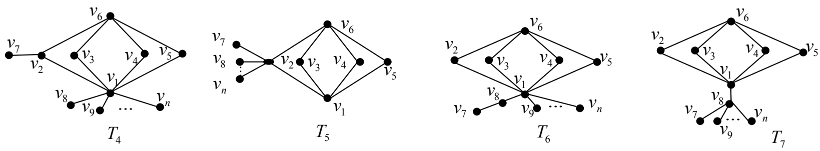

Figure 4. The graphs $T_j(j = 4, 5, 6, 7)$.

Lemma 4.1. *For the graphs T_4, T_5, T_6 and T_7 (as shown in Fig.4), T_4 is the one with maximum $EE(G)(EE_r(G), ER(G)$ or $Kf(\overline{G}))$.*

Proof. For the graph T_7, let $H_7 = T_7 - \{v_8v_9, \cdots, v_8v_n\}$. For any closed walk $W \in W_{2k}(H_7; v_8, v_8)$, if W does not reach the the vertex v_1, then let $f(W)$ be the walk obtained from W by replacing v_7 and v_8 by v_5 and v_1, respectively; Otherwise, W can be decomposed three sections W_1, W_2, W_3, denoted by $W = W_1W_2W_3$, where W_1 is the shortest (v_8, v_1)-section at the beginning of W, W_2 is the longest (v_1, v_1)-section of W, and W_3 is the remaining (v_1, v_8)-section. We will construct an injection f from $W_{2k}(H_7; v_8, v_8)$ to $W_{2k}(H_7; v_1, v_1)$. Let v_i be the predecessor of the last vertex v_1 on W_2, and v_j be a vertex taken from $\{v_2, v_3, v_4, v_5\}$ but distinct from v_i. We define $f_1(W_1)$ and $f_3(W_3)$ are the walk obtained from W_1 and W_3 by replacing v_8 and v_7 by v_j and v_6, respectively. Let $f(W) = W_2f_3(W_3)f_1(W_1)$, then $f(W) \in W_{2k}(H_7; v_1, v_1)$ and f is an injection. Further, $M_2(H_7; v_8, v_8) = 2 < 5 = M_2(H_7; v_1, v_1)$. Therefore $(H_7; v_8, v_8) \prec (H_7; v_1, v_1)$. Note that $T_6 = H_7 + \{v_1v_9, \cdots, v_1v_n\}$ and $T_7 = H_7 + \{v_8v_9, \cdots, v_8v_n\}$, by Lemma 2.5, we have $M_{2k}(T_7) < M_{2k}(T_6)$.

For the graph T_6, let $H_6 = T_6 - v_7v_8$, for any closed walk $W \in W_{2k}(H_6; v_8, v_8)$, let $W = v_8v_1W'v_1v_8$, where W' is the (v_1, v_1) closed walk of H_6. We let $f(W) = v_2v_1W'v_1v_2$, obviously, $f(W) \in W_{2k}(H_6; v_2, v_2)$ and f is an injection. By $M_2(H_6; v_8, v_8) = 1$, $M_2(H_6; v_2, v_2) = 2$, therefore $(H_6; v_8, v_8) \prec (H_6; v_2, v_2)$. Considering that $T_4 = H_6 + v_2v_7$ and $T_6 = H_6 + v_8v_7$, by Lemma 2.5, we have $M_{2k}(T_6) < M_{2k}(T_4)$.

For the graph T_5, let $H_5 = T_5 - v_2v_8, v_2v_9, \cdots, v_2v_n$, $H_5' = H_5 - v_1v_3$. Then there exists an automorphism σ of H_5' which interchange v_1 and v_2, and preserves all other vertices. By Lemma 2.7, We have $M_{2k}(H_5; v_2, v_2) < M_{2k}(H_5; v_1, v_1)$. Note that $T_4 = H_5 + \{v_1v_8, \cdots, v_1v_n\}$ and $T_5 = H_5 + \{v_2v_8, \cdots, v_2v_n\}$, by Lemma 2.5, we have $M_{2k}(T_5) < M_{2k}(T_4)$.

According to the same way, we can verify that $M_{2k}(S(T_4))$ is the biggest number among $M_{2k}(S(T_4))$, $M_{2k}(S(T_5))$, $M_{2k}(S(T_6))$, $M_{2k}(S(T_7))$. By Eqs.(1.1)-(1.3),(2.5), the lemma holds. ∎

Lemma 4.2. *If $G \in \mathcal{T}_n^+$ is the graph with the second maximum $EE(G)(EE_r(G), ER(G)$ or $Kf(\overline{G}))$ and $B(G) \cong A_1$, then $G \cong A_1(n-7,0,0,0,0,1)$.*

Proof. (i) For the case $A_1(n_1, n_2, 0, 0, 0, 0)$, let H be the graph obtained from it by deleting the edges v_3v_1, v_4v_1, $n_1 - 1$ pendent vertices attached at v_1 and $n_2 - 1$ pendent vertices attached at v_2. Then there exists an automorphism σ of H which interchange v_1 and v_2 and preserves other vertices. Let H' be the graph obtain from H by adding the edges v_3v_1, v_4v_1, $n_2 - 1$ pendent vertices attached at v_2. It is clear that $M_2(H'; v_2, v_2) = 3 < 4 + n_1 = M_2(H'; v_1, v_1)$. By Lemma 2.7 (ii), we have

$$(H'; v_2, v_2) \prec (H'; v_1, v_1) \ .$$

Further by Lemma 2.5, it follows that

$$M_{2k}(A_1(n_1, n_2, 0, 0, 0, 0)) \leq M_{2k}(A_1(n_1 + n_2 - 1, 1, 0, 0, 0, 0)) \ .$$

Let $T_4 = A_1(n-7, 1, 0, 0, 0, 0)$ and $T_3 = A_1(n-7, 0, 0, 0, 0, 1)$. We put H_1 be the graph obtained from T_4 by deleting the edges v_3v_6, v_4v_6 and the pendent vertex of v_2, and let $H_1' = H_1 + (v_3v_6, v_4v_6)$. There exists an automorphism σ' of H_1 such that $\sigma'(v_2) = v_6$. From Lemma 2.7 (ii), it follows that $(H_1'; v_2, v_2) \prec (H_1'; v_6, v_6)$. Then, by Lemma 2.5, we have $M_{2k}(T_4) \leq M_{2k}(T_3)$.

(ii) For the case $A_1(n_1, 0, 0, 0, 0, n_6)$, it is trifle for $n_1 = 1$ or $n_6 = 1$, thus we put $n_1 \geq 2, n_6 \geq 2$. Let $A = K_{1,n_1-1}, B = K_{1,n_6-1}$ and C be the graph obtained from $A_1(n_1, 0, 0, 0, 0, n_6)$ by deleting $n_1 - 1$ and $n_6 - 1$ pendent vertices of v_1 and v_6,respectively, by Lemma 2.6 (ii), it follows that

$$M_{2k}(A_1(n_1, 0, 0, 0, 0, n_6)) \leq M_{2k}(T_3) \ .$$

Therefor, the Lemma is true for the indices $EE(G)$,$EE_r(G)$ and $ER(G)$.

By a similar discussion mentioned above, we can show that $Kf(\overline{G}) \leq Kf(\overline{T_3})$, which is omitted here. ■

From Theorem 3.9 and Lemma 4.2, we obtain the following corollary.

Corollary 4.3. *If $G \in \mathcal{T}_n^+$ is the graph with the second maximum $EE(G)(EE_r(G)$, $ER(G)$ or $Kf(\overline{G}))$, then $G \in \{T_2, T_3\}$.*

By Lemma 2.3, we calculate the characteristic polynomial of T_3 as the following

$$\phi(T_3; x) = x^{n-4}[x^4 - (n+2)x^2 + 5n - 31] = x^{n-4} f_3(x)$$

From Lemma 2.3 and the equation 2.5, it follows that

$$\begin{aligned}\sigma(T_3;x) &= x(x-1)^{n-8}[x^7-(n+12)x^6+(14n+44)x^5-(72n+40)x^4\\ &+ (180n-96)x^3-(232n-24)x^2+(144n-128)x-32n]\\ &= x(x-1)^{n-8}g_3(x)\ .\end{aligned}$$

Theorem 4.4. *Let G be a bipartite tricyclic graph with $n \geq 8$, and $G \ncong T_1$, then (i) $EE(G) \leq EE(T_2)$, $Kf(\overline{G}) \leq Kf(\overline{T_2})$ with equality if and only if $G \cong T_2$. (ii) $ER(G) \leq ER(T_3)$ and $EE_r(G) \leq EE_r(T_3)$ with equality if and only if $G \cong T_3$.*

Proof. (i) By Corollary 4.2, we just determine the graph between T_2 and T_3. By calculation using software Matlab, we have $EE(T_2) > EE(T_3)$ when $8 \leq n \leq 35$. In the following discussion, we let $n \geq 36$.

The solutions of $f_3(x)=0$ are $\pm\sqrt{\frac{n+2+\sqrt{n^2-24n+128}}{2}}, \pm\sqrt{\frac{n+2-\sqrt{n^2-24n+128}}{2}}$ and the graph $T_3 - v_1$ has eigenvalues $\pm\sqrt{5}$, 0 with multiplicity $n-3$. By interlacing property of eigenvalues of $T_3 - v_1$ and T_3, $\lambda_i(T_3) \leq \lambda_{i-1}(T_3 - v_1)$ for $i = 2,3,\ldots,n$ [3]. Then

$$\begin{aligned}EE(T_3) &= \sum_{i=1}^{n} e^{\lambda_i(T_3)} \leq e^{\lambda_1(T_3)} + \sum_{i=2}^{n} e^{\lambda_{i-1}(T_3-v_1)}\\ &= e^{\sqrt{\frac{n+2+\sqrt{n^2-24n+128}}{2}}} + (n-3) + e^{\sqrt{5}} + e^{-\sqrt{5}}\\ &< e^{\sqrt{\frac{n+2+\sqrt{n^2-23n+132.25}}{2}}} + (n-3) + e^{\sqrt{5}} + e^{-\sqrt{5}}\\ &= e^{\sqrt{n-\frac{19}{4}}} + (n-3) + e^{\sqrt{5}} + e^{-\sqrt{5}}\end{aligned}$$

For $n \geq 36$,

$$f_2(\sqrt{n-3}) = -13n-45 < 0, \qquad f_2(\sqrt{n-\frac{5}{2}}) = \frac{1}{2}(n^2-36n+\frac{391}{4}) > 0$$

we have $\lambda_1(T_2) > \sqrt{n-3}$. The graph $T_2 - v_1$ has eigenvalues $\pm\sqrt{\frac{5+\sqrt{17}}{2}}, \pm\sqrt{\frac{5-\sqrt{17}}{2}}$, 0 with multiplicity $n-5$, by interlacing property of eigenvalues of $T_2 - v_1$ and T_2, $\lambda_i(T_2) \geq \lambda_i(T_2 - v_1)$ for $i = 2,3,\ldots,n-1$, then

$$\begin{aligned}EE(T_2) &= \sum_{i=1}^{n} e^{\lambda_i(T_2)} \geq e^{\lambda_1(T_2)} + \sum_{i=2}^{n-1} e^{\lambda_i(T_2-v_1)}\\ &> e^{\sqrt{n-3}} + (n-5) + e^{-\sqrt{\frac{5+\sqrt{17}}{2}}} + e^{\sqrt{\frac{5-\sqrt{17}}{2}}} + e^{-\sqrt{\frac{5-\sqrt{17}}{2}}}.\end{aligned}$$

Note that $e^{\sqrt{n-3}} - e^{\sqrt{n-\frac{9}{4}}} > 2 + e^{\sqrt{5}}$ for $n \geq 22$, then $EE(T_2) > EE(T_3)$.

According to the way mentioned above, we have

$$\begin{aligned}Kf(\overline{T_3}) - Kf(\overline{T_2}) &= n\left(\frac{\sigma'(T_3,n)}{\sigma(T_3,n)} - \frac{\sigma'(T_2,n)}{\sigma(T_2,n)}\right)\\ &= \frac{n^2(-n^9+145n^8-1203n^7+3511n^6+\cdots+864)}{(n-1)g_3(n)g_2(n)}\end{aligned}$$

Because of the fact that the denominator is positive and the numerator is negative on $n \geq 8$, it follows that $Kf(\overline{T_2}) > Kf(\overline{T_3})$.

(ii) By Lemma 2.1, we have

$$\begin{aligned} ER(T_3) - ER(T_2) &= \frac{\phi'(T_3,n)}{\phi(T_3,n)} - \frac{\phi'(T_2,n)}{\phi(T_2,n)} \\ &= \frac{20n^6 - 22n^5 + 60n^4 - 32n^3 - 116n^2 + 244n - 744}{nf_2(n)f_3(n)} \end{aligned}$$

The real roots of the polynomials $f_3(n) = n^4 - n^3 - 2n^2 + 5n - 31$ and $f_2(n) = n^6 - n^5 - 2n^4 + 5n^3 - 26n^2 - 2n + 12$ are less than 3, thus the denominator is positive on $n \geq 3$. On the other hand, the polynomial $p(n) = 20n^6 - 22n^5 + 60n^4 - 32n^3 - 116n^2 + 244n - 744$ is positive on $n \geq 3$. It implies that $ER(T_3) > ER(T_2)$.

Similarly, by Lemma 2.1, it follows that

$$\begin{aligned} EE_r(T_3) - EE_r(T_2) &= (n-1)\left(\frac{\phi'(T_3,n-1)}{\phi(T_3,n-1)} - \frac{\phi'(T_2,n-1)}{\phi(T_2,n-1)}\right) \\ &= \frac{20n^6 - 142n^5 + 448n^4 - 788n^3 + 656n^2 + 54n - 768}{f_1(n-1)f_2(n-1)} \end{aligned}$$

the numerator is positive for $n \geq 4$, and the real roots of the polynomials $f_1(n-1)$ and $f_2(n-1)$ are less than 4, thus the valuation of the fraction is positive for $n \geq 4$. It follows that $EE_r(T_3) \geq EE_r(T_2)$. ■

Remark 3. We would like to point out that the set $\mathcal{T}_n^+$ is a special case of the set $\mathcal{T}_n^c (c = 0, 1, 2, 3 \cdots)$, i.e. the set of connected bipartite c-cyclic graphs. The extremal bipartite c-cyclic graphs for $c = 0, 1, 2$ have been characterized according to the Estrada index, for the details, the readers may refer to [15,20,32]. For solving the same problem on the set $\mathcal{T}_n^c, c \geq 4$, our approach would need to be modified, it would be interesting to continue studying the extremal graphs.

References

[1] B. Bollobás, *Modern Graph Theory*, Springer–Verlag, Berlin, 1998.

[2] N. L. Biggs, *Algebraic Graph Theory*, Cambridge Univ. Press, Cambridge, 1993.

[3] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.

[4] H. Zhu, D.J. Klein, I. Lukovits, Extensions of the Wiener number, *J. Chem. Inf. Comput. Sci.* **36** (1996) 420–428.

[5] D. J. Klein, M. Randić, Resistance distance, *J. Math. Chem.* **12** (1993) 81–95.

[6] P. Csikvári, On a poset of trees, *Combinatorica* **30** (2010) 125–137.

[7] D. Bonchev, A. T. Balaban, X. Liu, D. J. Klein, Molecular cyclicity and centricity of polycyclic graphs. I. Cyclicity based on resistance distances or reciprocal distances, *Int. J. Quantum Chem.* **50** (1994) 1–20.

[8] Z. Du, Z. Liu, On the Estrada and Laplacian Estrada indices of graphs, *Lin. Algebra Appl.* **435** (2011) 2065–2076.

[9] J. Zhang, B. Zhou, J. Li, On Estrada index of trees, *Lin. Algebra Appl.* **434** (2011) 215–223.

[10] B. Zhou, On Estrada index, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 485–492.

[11] I. Gutman, B. Mohar, The quasi–Wiener and the Kirchhoff indices coincide, *J. Chem. Inf. Comput. Sci.* **36** (1996) 982–985.

[12] I. Gutman, B. Furtula, E. Zogić, E. Glogić, Resolvent energy of graphs, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 279–290.

[13] K. C. Das, K. Xu, I. Gutman, Comparison between Kirchhoff index and the Laplacian-energy-like invariant, *Lin. Algebra Appl.* **436** (2012) 3661–3671.

[14] K. C. Das, A. D. Güngör, A. Ş. Civik, On the Kirchhoff index and the resistance–distance energy of a graph, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 541–556.

[15] Q. Deng, H. Chen, On extremal bipartite unicyclic graphs, *Lin. Algebra Appl.* **444** (2014) 89–99.

[16] Q. Deng, H. Chen, On the Kirchhoff index of the complement of a bipartite graph, *Lin. Algebra Appl.* **439** (2013) 167–173.

[17] A. Ilić, D. Stevanović, The Estrada index of chemical trees, *J. Math. Chem.* **47** (2010) 305–314.

[18] L. Wang, Y. Z. Fan, Y. Wang, Maximum Estrada index of bicyclic graphs, *Discr. Appl. Math.* **180** (2015) 194–199.

[19] X. Chen, J. Qian, On resolvent Estrada index, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 163–174.

[20] J. Huang, S. Li, Q. Zhao, On extremal bipartite bicyclic graphs, *J. Math. Anal. Appl.* **436** (2016) 1242–1255.

[21] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713–718.

[22] E. Estrada, Characterization of the folding degree of proteins, *Bioinformatics* **18** (2002) 697–704.

[23] E. Estrada, Topological structural classes of complex networks, *Phys. Rev. E* **75** (2007) 016103.

[24] E. Estrada, Characterization of the amino acid contribution to the folding degree of proteins, *Proteins* **54** (2004) 727–737.

[25] E. Estrada, J. A. Rodríguez–Valázquez, Subgraph centrality in complex networks, *Phys. Rev. E* **71** (2005) 0561031.

[26] E. Estrada, D. J. Higham, Network properties revealed through matrix functions, *SIAM Rev.* **52** (2010) 696–714.

[27] E. Estrada, N. Hatano, Topological atomic displacements, Kirchhoff and Wiener indices of molecules, *Chem. Phys. Lett.* **486** (2010) 166–170.

[28] E. Estrada, J. A. Rodríguez–Valázquez, M. Randić, Atomic branching in molecules, *Int. J. Quantum Chem.* **106** (2006) 823–832.

[29] Y. Yang, Bounds for the Kirchhoff index of bipartite graphs, *J. Appl. Math.* (2012) 195242.

[30] S. Li, X. Li, Z. Zhu, On tricyclic graphs with minimal energy, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 397–419.

[31] Z. Zhu, L. Tan, Z. Qiu, Tricyclic graph with maximal Estrada index, *Discr. Appl. Math.* **162** (2014) 364–372.

[32] H. Zhou, Y. Jia, On the Estrada index of bipartite graph, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 495–501.